Sebacic acid, 4-bromo-2,6-difluorobenzyl butyl ester

Inchi: InChI=1S/C21H29BrF2O4/c1-2-3-12-27-20(25)10-8-6-4-5-7-9-11-21(26)28-15-17-18(23)
InchiKey: UJTAWZADDNDVPA-UHFFFAOYSA-N
Formula: C21H29BrF2O4
SMILES: CCCCOC(=O)CCCCCCCCC(=O)OCc1c(F)cc(Br)cc1F
Mol. weight [g/mol]: 463.35

Physical Properties

Property code	Value	Unit	Source
gf	-633.68	kJ/mol	Joback Method
hf	-1130.14	kJ/mol	Joback Method
hfus	60.04	kJ/mol	Joback Method
hvap	89.72	kJ/mol	Joback Method
log10ws	-7.76		Crippen Method
logp	6.235		Crippen Method
mcvol	318.910	ml/mol	McGowan Method
pc	1208.15	kPa	Joback Method
rinpol	2779.00		NIST Webbook
rinpol	2779.00		NIST Webbook
tb	938.78	K	Joback Method
tc	1150.07	K	Joback Method
tf	595.71	K	Joback Method
vc	1.250	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.80	J/mol×K	938.78	Joback Method
cpg	1003.78	J/mol×K	973.99	Joback Method
cpg	1016.57	J/mol×K	1009.21	Joback Method
cpg	1028.20	J/mol×K	1044.42	Joback Method
cpg	1038.69	J/mol×K	1079.64	Joback Method
cpg	1048.07	J/mol×K	1114.85	Joback Method
cpg	1056.38	J/mol×K	1150.07	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380807&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume